

Evaluation of
Calpuff Model Performance
Using Year 2000 Data

Draft

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Introduction

Performance of the Calpuff model (Version 5.4, Level 000602_1), as implemented by the North Dakota Department of Health (NDDH) for Year 2000 data, was evaluated using SO₂ observations from the NDDH Dunn Center and Theodore Roosevelt National Park (TRNP) South Unit monitoring sites. Meteorological input data for Calpuff were developed using the Calmet meteorological model (Version 5.2, Level 000602a). Source emission rates were based on CEM's hourly data (where available) or annual average emission for Year 2000.

The performance evaluation proceeded in an iterative manner to determine the effect of adjustments to settings in the Calmet and Calpuff input control files on model skill. The majority of these settings were left equivalent to recommendations in "IWAQM Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts," 1998. But changes to a limited number of settings were judged to be scientifically advantageous for the region of model application, and resulted in improved model agreement with observations. A single Calpuff receptor was included for each monitoring site.

The iterative procedure resulted in a final set of Calmet/Calpuff input conditions which yielded very good agreement with observations. All of the predicted/observed ratios fell within the factor-of-two criteria suggested by EPA.

Source Inventory

The evaluation analysis accounted for all SO₂ sources located within a reasonable distance of the two monitoring sites, and which operated during Year 2000. The inventory included all significant SO₂ sources within 250 km of the sites. Oil and gas production sources (i.e., treaters and flares) were also included. But because of their greater number and smaller size, the modeled inventory of oil and gas sources was limited to those located within 50 km of each monitoring site.

SO₂ sources included in the evaluation analysis are identified in Table 1. Source locations with respect to monitoring sites are depicted in Figure 1 (oil and gas source locations not shown).

SO₂ emission rates and stack operating parameters (i.e., exit velocity and temperature) were based on CEM's hourly data for Year 2000 where available. For significant sources with no CEM's data, constant emission rates and operating parameters reflecting annual

average operation for Year 2000 were utilized. Annual average stack data for oil and gas production sources were derived from monthly production data for Year 2000. The emission characterization for each source is indicated in Table 1. As shown in Table 1, hourly emissions data were available for a majority of significant sources, and for most of the largest sources.

Emission rates for oil and gas production sources were derived from the ND State Industrial Commission's Oil and Gas data base. The oil and gas sources were screened to eliminate those with zero or minimal emissions. Stack operating parameters for oil and gas production sources were derived using procedures described in the "Williston Basin Regional Air Quality Study" (1990), and modified using SCREEN3 (EPA screening model) adjustments for effective flare plume height and radiational heat loss.

Calmet Input Data

The location of the 10 km computational grid utilized by the NDDH for the Year 2000 analysis is represented in Figure 1. The grid is defined by eight vertical layers. Meteorological input data for Calmet was based on 32 surface stations, 5 upper-air stations, and 89 precipitation stations located in or near the computational grid. GOES ASOS satellite data were used to supplement surface observations for ceiling height and sky cover. All meteorological data were obtained from the National Climatic Data Center (surface and precipitation data), or Forecast Systems Laboratory (upper-air data). Geophysical data were developed using the USGS GTOPO30 data set for terrain elevations and the USGS Global data set for land use.

Processing of meteorological data relied on Earth Tech software, as well as supplemental software developed by NDDH for format conversions and missing data substitution. Methodology for meteorological data preparation is generally consistent with that described in "Calpuff Class I Area Analysis for Milton R. Young Generating Station" (Draft), 1999. That methodology was modified for the Year 2000 analysis largely because of the inclusion of GOES ASOS satellite data. Methodology specific to the Year 2000 analysis has been informally described, and will be formally documented in a future report. Note that the possibility/effect of alternative approaches to meteorological data preparation was not considered in the performance evaluation.

Processing of terrain and land use data was strictly objective, and relied exclusively on Earth Tech software. Note that the seasonal

scheme for land use related parameters, which has been informally documented, is not incorporated in the final iteration of the performance evaluation, which provided the best agreement with observations. Rather, Calmet default parameters were assumed for the entire year.

Calmet/Calpuff Control File Settings

For the most part, Calmet and Calpuff input control file settings, as implemented by the NDDH, were consistent with IWAQM recommendations. However, extensive testing of Calmet output, with visual feedback (plotted data), suggested that adjustment to a limited number of IWQAM settings was required to achieve reasonable results for wind and mixing height fields. Further, the adjustment of a limited number of additional settings was found to provide better agreement with observations in the performance evaluation, and such changes were judged to be scientifically consistent.

Non-IWAQM settings utilized by the NDDH for Calmet and Calpuff control files, and which provided optimum agreement with monitored observations, are listed in Table 2. These Non-IWAQM settings are discussed below.

Calmet

IKINE - The inclusion of kinematic effects provided significantly better agreement of Calpuff results with monitored observations. From a scientific standpoint, it seems inconsistent for IWAQM to recommend wind adjustment using Froude number effects (IFRADJ), and not kinematic effects.

BIAS(NZ) - NDDH bias settings were developed through significant testing with visual feedback. The IWAQM recommendation provides neutral bias (between surface and upper-air data) for all vertical layers. In light of its testing, the NDDH does not believe it is reasonable to assume equal weighting of upper-air wind data with surface data at the lowest level, and to assume equal weighting of surface data with upper-air data at top levels.

LVARY - The NDDH felt it necessary to deploy this option to ensure that at least one station would always be available.

ZUPWND(2) - The NDDH was concerned that IWAQM was recommending a value of 1000 m while the model (Earth Tech) default is

2500 m, thus prompting the NDDH compromise value of 2000 m. But regardless of the selected value for this initial guess wind field input, subsequent wind field development should converge to the same result.

MNMDAV/ILEVZI - The NDDH found that IWAQM default values for these parameters, relating to spatial averaging of mixing heights, produced entirely unacceptable results for the mixing height field. Severe gradients (bull's eyes) in mixing height were observed in the immediate vicinity of meteorological stations, and a significant increase in the value of these input parameters was required to mitigate the anomaly. The NDDH notes that because MNMDAV is a function of grid cell size, IWAQM should specify "User Defines" for this parameter.

ZIMAX/ZIMAXW - Because the NDDH Calmet, Calpuff grid extends into the western part of the upper Great Plains, maximum mixing height was increased to 2000 m to be consistent with maximum mixing heights reported for this region (Holzworth, 1972).

Calpuff

MSPLIT - The option for puff splitting was recommended by John Irwin (EPA) when modeling source-receptor distances of 200 km or more, because of the tendency for Calpuff to otherwise overpredict at these distances. Deployment of this option also provided better agreement with observations.

MDISP - Use of dispersion coefficient option 2 provided significantly better agreement with observations. The NDDH also believes this selection is more consistent with the "state-of-the-art" in air quality modeling.

BCKO3 - Though the NDDH is utilizing the hourly file option for ozone background, the BCKO3 value is substituted by Calpuff when hourly data are missing. Based on local monitoring data, NDDH judged the IWQAM value of 80 ppb to be much higher than typical for North Dakota, and therefore reset the value to 30 ppb.

BCKNH3 - The NDDH value of 2 ppb reflects the annual average of local, unbiased monitoring data.

XSAMLEN - The NDDH set this value lower than the IWAQM recommendation, but notes that the only consequence for doing

so would be extra computer time due to more puffs on the grid.

The goal was to improve model resolution by increasing the number of puffs and decreasing mass per puff. Again, because this parameter is a function of grid cell size, the NDDH believes the recommended XSAMLEN value should be "User Defined".

XMAXZI - Value was increased to 4000 m for consistency with ZIMAX/ZIMAXW setting in Calmet.

Some other deviations from IWAQM guidance, which had no consequence for model predictions, were also involved in the NDDH implementation. These related to printed output options and parameters for the Lambert conformal map projection used by the NDDH.

Results

Results of the performance evaluation are summarized in Figure 2 for the Dunn Center monitoring site and in Figure 3 for the TRNP South monitoring site. The Figures include quantile-quantile plots of the highest 50 predictions and observations for 3-hour and 24-hour averaging times. The plots include "factor-of-two" curves for assessing performance. Note that these results represent the final iteration of the performance evaluation process, as reflected by the control file settings in Table 2.

Inspection of the quantile-quantile plots in Figures 2 and 3 reveals that the capability of the NDDH Calpuff modeling system to reproduce observed SO₂ concentrations is very good. All predicted-to-observed ratios fall within the factor-of-two criteria suggested by EPA, and in most cases are much better. Though some of the 50 highest 24-hour averages at both monitoring sites were underpredicted, it appears the modeling system produces no systematic bias toward underprediction or overprediction when considering the ensemble results.

One caveat regarding these results is that TRNP South Unit monitoring data for Year 2000 included extensive missing periods (about 700 hours total). Therefore, maximum observations may be under-represented in the comparative analysis, moving the bias more toward underprediction, particularly for 24-hour averages.

Conclusions

The evaluation of Calpuff performance for Year 2000 data at Dunn Center and TRNP South Unit monitoring sites indicates the modeling system performs well, when implemented using IWAQM control file settings as modified by NDDH (Table 2). Predicted-to-observed ratios for the fifty highest predicted/observed concentrations fell within the factor-of-two criteria suggested by EPA, and did not exhibit systematic bias toward underprediction or overprediction. Therefore, the NDDH implementation of the Calpuff modeling system, using currently processed meteorological/geophysical data and IWAQM control file settings as modified by NDDH, should be acceptable for regulatory Class I area modeling in North Dakota.

The NDDH recognizes that minor improvement in model performance is still possible. But the implication of these performance evaluation results is that caution must attend any suggested changes to input or methodology. Changing all control file settings to IWAQM-recommended values, for example, would likely move some predicted-to-observed ratios outside of the factor-of-two window.

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Table 1
Source Inventory (SO₂)

Source	Emission Characterization	Figure 1 Loc. Key
Coal Creek Station	Actual Hourly	1
Antelope Valley Station	Actual Hourly	2
Coyote Station	Actual Hourly	3
Leland Olds Station	Actual Hourly	4
Milton R. Young Station	Actual Hourly	5
Heskett Station	Actual Hourly	6
Stanton Station	Actual Hourly	4
Great Plains Synfuels Plant	Actual Hourly*	2
Little Knife Gas Plant	Actual Hourly	7
Grasslands Gas Plant	Actual Hourly	8
Tioga Gas Plant	Annual Average	9
Lignite Gas Plant	Annual Average	10
Mandan Refinery	Annual Average	6
Boundary Dam Station	Annual Average	11
Shand Station	Annual Average	12
Colstrip Station	Actual Hourly	13
CELP Boiler	Annual Average	14
Sidney Station	Annual Average	15
Oil & Gas Related**	Annual Average	—

* Hourly CEM's data were available for GPSP main stack only. Annual average emission assumed for other three units.

** All facilities located within 50 km of monitoring sites.

Table 2
Non-IWAQM Settings Used by NDDH
in Calmet/Calpuff Control Files

Parameter	IWAQM	NDDH
<u>Calmet</u>		
IKINE	0	1
BIAS (NZ)	0,0,0,0, 0,0,0,0	-1.0, -0.9, -0.7, 0.0, 0.5, 1.0, 1.0, 1.0
LVARY	F	T
ZUPWND (2)	1000 m	2000 m
MNMDAV	1	8
ILEVZI	1	4
ZIMAX	2000 m	4000 m
ZIMAXW	3000 m	4000 m
<u>Calpuff</u>		
MSPLIT*	0	1
MDISP	3	2
BCKO3	80 ppb	30 ppb
BCKNH3	10 ppb	2 ppb
XSAMLEN	1.0	0.5
XMAXZI	3000 m	4000 m

* Puff splitting was not deployed in Calpuff control file for oil and gas sources. This concession to model execution time is reasonable, because puffs would not grow very large given the maximum 50 km source-receptor distance.

Figure 1: Monitor and Source Locations

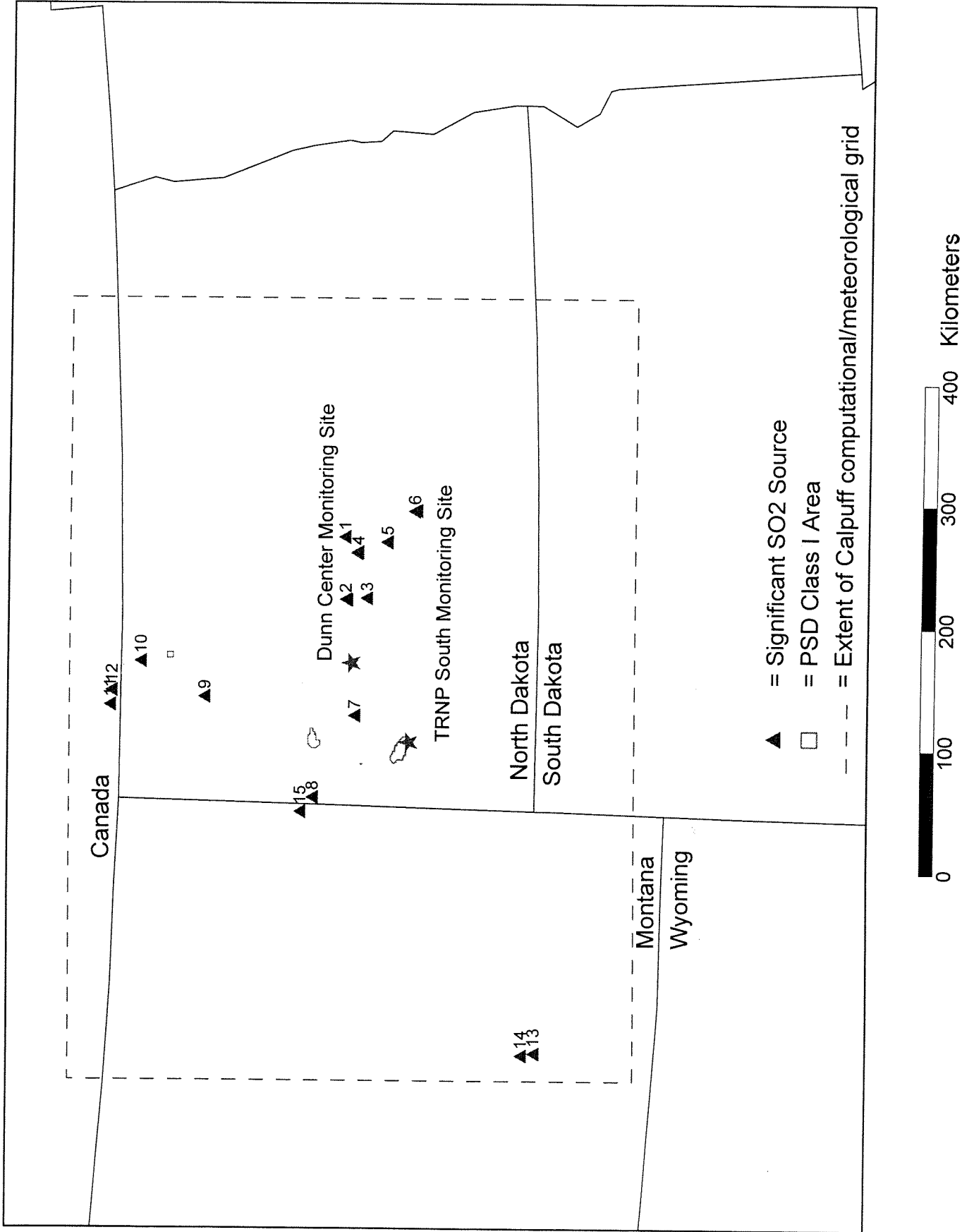


Figure 2

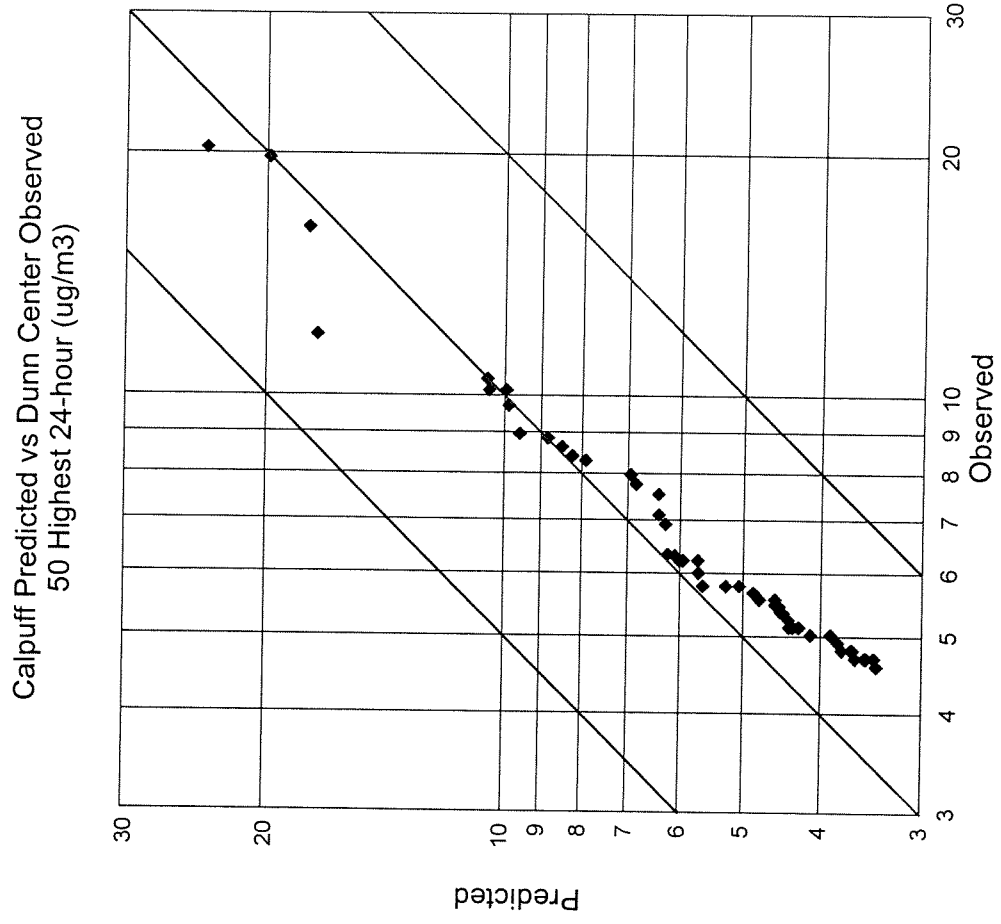
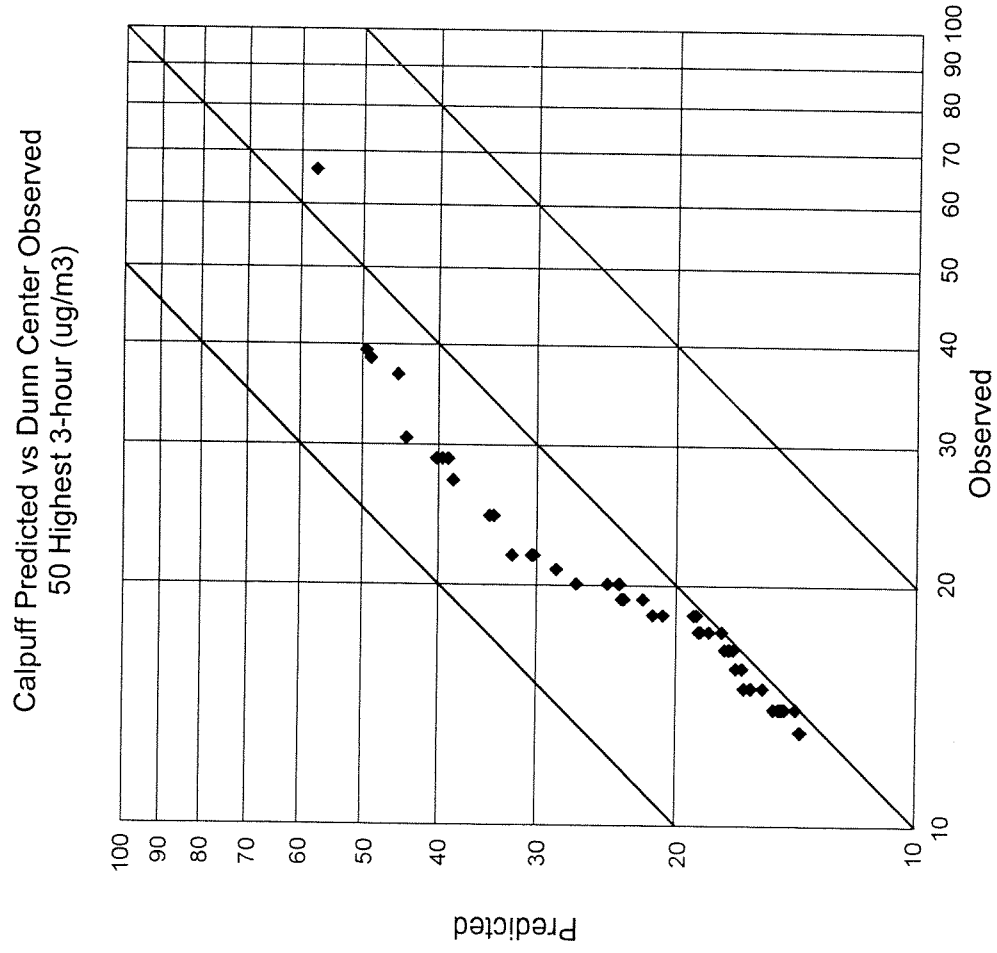
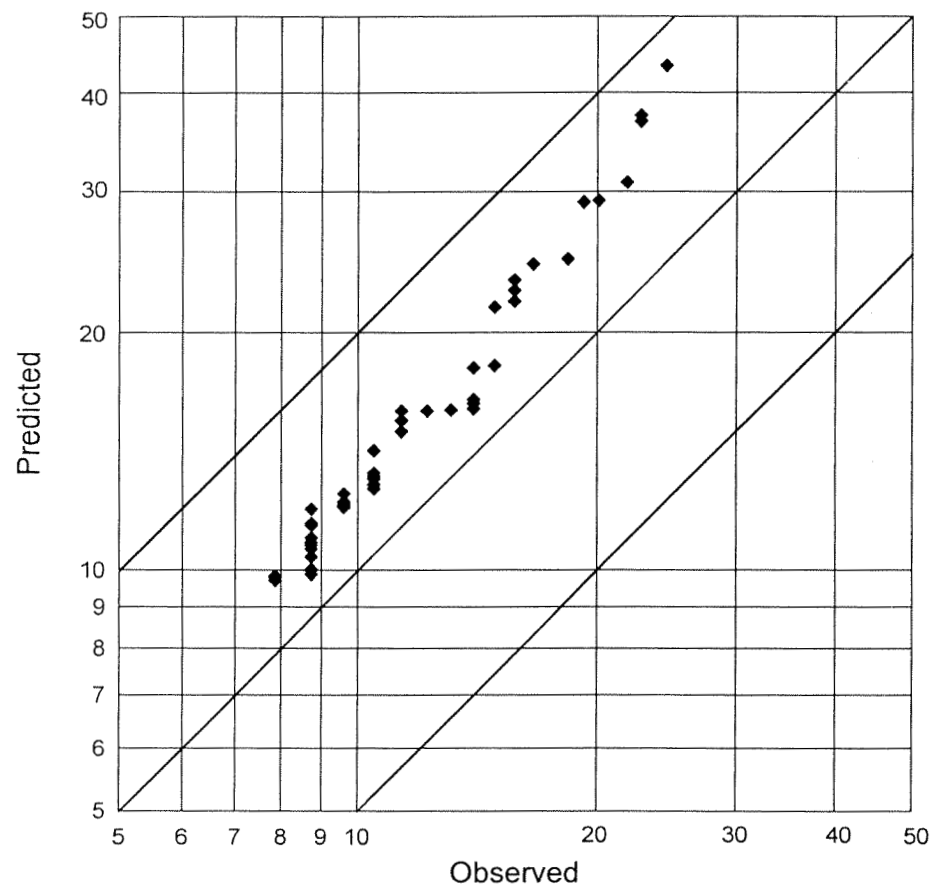


Figure 3

Calpuff Predicted vs TR South Observed
50 Highest 3-hour (ug/m3)



Calpuff Predicted vs TR South Observed
50 Highest 24-hour (ug/m3)

